

Transfer matrices for piecewise constant potentials

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By expressing the time-independent Schrödinger equation in one dimension as a system of two first-order differential equations, the transfer matrix for a rectangular potential barrier is obtained making use of the matrix exponential. It is shown that the transfer matrix allows one to find the bound states and the quasinormal modes. A similar treatment for the one-dimensional propagation of electromagnetic waves in a homogeneous medium is also presented.

Keywords: Scattering; transfer matrix; quasinormal modes; layered systems

Expresando la ecuación de Schrödinger independiente del tiempo en una dimensión como un sistema de dos ecuaciones diferenciales de primer orden, se obtiene la matriz de transferencia para una barrera de potencial rectangular haciendo uso de la exponencial de matrices. Se muestra que la matriz de transferencia permite hallar los estados ligados y los modos cuasinormales. Se presenta también un tratamiento similar para la propagación unidimensional de ondas electromagnéticas en un medio homogéneo.

Descriptores: Dispersión; matriz de transferencia; modos cuasinormales; sistemas en capas

PACS: 03.65.-w, 02.10.Ud

1. Introduction

A standard problem in elementary quantum mechanics is that of finding the reflection and transmission amplitudes for the scattering produced by a potential barrier, or well, in one dimension (see, *e.g.*, Refs. 1–4). The reflection and transmission amplitudes are conveniently arranged in the transfer matrix, which relates the wave function at both sides of the potential barrier, in such a way that the effect of two or more potential barriers is readily obtained by means of the product of the corresponding transfer matrices (see, *e.g.*, Ref. 5 and the references cited therein). A similar result applies for the one-dimensional propagation of electromagnetic waves in layered media (see, *e.g.*, Ref. 6). In fact, the transfer matrices can be defined in all cases where there is an output that depends linearly on an input; some important examples, apart from the two already mentioned, are the electric circuits and optical systems. In the cases considered here, the transfer matrices are 2×2 complex matrices but, depending on the equations involved (more specifically, the number of variables and the differential order), the size of the transfer matrices do vary.

The aim of this paper is to show that the transfer matrix for a rectangular potential barrier (and, therefore, for a piecewise constant potential) can be easily obtained integrating the time-independent Schrödinger equation in one dimension by means of the matrix exponential. The time-independent Schrödinger equation in one dimension, being a second-order ordinary differential equation, is equivalent to a system of two coupled first-order differential equations and, only in the case of a (piecewise) constant potential, this system can be easily integrated using the matrix exponential. We also show that making use of the transfer matrix one can find the bound states and the quasinormal modes. The transfer matrix for the one-dimensional propagation of electromagnetic waves in a medium with a piecewise constant refractive index is obtained in a similar manner, without employing the Fresnel coefficients.

In Sec. 2 an elementary discussion about the transfer matrices for the one-dimensional Schrödinger equation is given (see also Ref. 5 and the references cited therein). In Sec. 3 the transfer matrix for a rectangular barrier is obtained making use of the matrix exponential; the bound states and quasinormal modes are then found starting from the transfer matrix. In Sec. 4 a similar derivation for the case of the one-dimensional propagation of electromagnetic waves in layered media is given.

2. Transfer matrices

The solutions of the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \quad (1)$$

with a given short-range potential $V(x)$, which vanishes outside the interval $a \leq x \leq b$, can be expressed in the form

$$\psi(x) = \begin{cases} A_1 e^{ik(x-a)} + A_2 e^{-ik(x-a)}, & \text{for } x < a, \\ B_1 e^{ik(x-b)} + B_2 e^{-ik(x-b)}, & \text{for } x > b, \\ u(x), & \text{for } a \leq x \leq b, \end{cases} \quad (2)$$

where $k \equiv \sqrt{2mE}/\hbar$, A_1 , A_2 , B_1 , B_2 are constants and $u(x)$ is a function that depends on the explicit form of the potential $V(x)$. By imposing the usual conditions of continuity of $\psi(x)$ and its derivative at $x = a$ and $x = b$, a linear relation of the form

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = M \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} \quad (3)$$

can be obtained, where M is some 2×2 complex matrix (the transfer matrix), which depends on $V(x)$ and the value of k .

Assuming that $V(x)$ is real, Eq. (1) implies that the probability current density

$$j(x) = \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right),$$

where $*$ denotes complex conjugation, satisfies the continuity equation, $dj/dx = 0$, that is, $j(x) = \text{const.}$; then, making use of Eq. (2), one finds that, for k real

$$|A_1|^2 - |A_2|^2 = |B_1|^2 - |B_2|^2. \quad (4)$$

Using the fact that

$$|A_1|^2 - |A_2|^2 = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix},$$

where the † denotes the Hermitian adjoint, and Eq. (3) one finds that Eq. (4) is equivalent to

$$M^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (5)$$

The complex 2×2 matrices satisfying Eq. (5) form a group with the usual matrix multiplication (see below). Equation (5) implies that the modulus of $\det M$ is equal to 1.

The entries of the transfer matrix are related to the reflection and transmission amplitudes of the potential $V(x)$, denoted by r and t , respectively. When there are no waves coming from the right ($B_2 = 0$), there exist solutions of the Schrödinger equation of the form

$$\psi(x) = \begin{cases} e^{ik(x-a)} + re^{-ik(x-a)}, & \text{for } x < a, \\ te^{ik(x-b)}, & \text{for } x > b, \\ u_1(x), & \text{for } a \leq x \leq b, \end{cases} \quad (6)$$

that is, solutions of the form (2) with $A_1 = 1$, $A_2 = r$, and $B_1 = t$. Thus, from Eq. (3) it follows that

$$M = \begin{pmatrix} 1/t & M_{12} \\ r/t & M_{22} \end{pmatrix},$$

with M_{12} and M_{22} not yet identified, and from Eq. (4) we obtain the well-known relation

$$1 - |r|^2 = |t|^2. \quad (7)$$

(In most textbooks the reflection and transmission amplitudes are defined by means of expressions similar to Eq. (6), with r and t being the coefficients of e^{-ikx} and e^{ikx} and therefore, the amplitudes r and t defined by Eq. (6) differ from those usually employed by factors e^{ika} and e^{-ikb} , respectively.)

Since $V(x)$ is real, for k real the complex conjugate of the solution (6)

$$\psi^*(x) = \begin{cases} r^*e^{ik(x-a)} + e^{-ik(x-a)}, & \text{for } x < a, \\ t^*e^{-ik(x-b)}, & \text{for } x > b, \\ u_1^*(x), & \text{for } a \leq x \leq b, \end{cases} \quad (8)$$

is also a solution of the Schrödinger equation. Substituting the coefficients appearing in Eq. (8) into Eq. (3) we find that

$$M = \begin{pmatrix} 1/t & r^*/t^* \\ r/t & 1/t^* \end{pmatrix}. \quad (9)$$

Then, according to Eq. (7), $\det M = 1$, which means that (for k real) the transfer matrix belongs to the group $SU(1,1)$, formed by the 2×2 complex matrices with unit determinant that satisfy Eq. (5).

The reflection and transmission amplitudes of the potential $V(x)$ for waves incident from the right, r' and t' , respectively, need not coincide with r and t . In fact, from Eqs. (3) and (9), setting

$A_1 = 0$ and $B_2 = 1$, we must have

$$\begin{pmatrix} 0 \\ t' \end{pmatrix} = \begin{pmatrix} 1/t & r^*/t^* \\ r/t & 1/t^* \end{pmatrix} \begin{pmatrix} r' \\ 1 \end{pmatrix},$$

which, making use of Eq. (7), implies that

$$t' = t, \quad 0 = \frac{r'}{t} + \frac{r^*}{t^*}. \quad (10)$$

Hence, $r = r'$ if and only if r/t is pure imaginary.

3. Rectangular barriers

The reflection and transmission amplitudes for a given potential are usually obtained by solving the time-independent Schrödinger equation (1) (see, *e.g.*, Refs. 1–4). In the exceptional case of a piecewise constant potential, the transfer matrix (and, therefore, the reflection and transmission amplitudes) can be readily obtained by means of matrix exponentiation.

The time-independent Schrödinger equation (1) can be expressed as the first-order differential equation

$$\frac{d}{dx} \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ v(x) - k^2 & 0 \end{pmatrix} \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix}, \quad (11)$$

where $v(x) \equiv 2mV(x)/\hbar^2$. Hence, if $V(x)$ is a constant V_0 for $a \leq x \leq b$, the solution of Eq. (11) is

$$\begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} = \exp \left[x \begin{pmatrix} 0 & 1 \\ v_0 - k^2 & 0 \end{pmatrix} \right] \begin{pmatrix} c_1 \\ c_2 \end{pmatrix},$$

for $a \leq x \leq b$, where $v_0 \equiv 2mV_0/\hbar^2$, and c_1, c_2 are some constants. Thus,

$$\begin{pmatrix} \psi(a) \\ \psi'(a) \end{pmatrix} = \exp \left[-L \begin{pmatrix} 0 & 1 \\ v_0 - k^2 & 0 \end{pmatrix} \right] \begin{pmatrix} \psi(b) \\ \psi'(b) \end{pmatrix}, \quad (12)$$

with $L \equiv b - a$. Letting

$$J \equiv \begin{pmatrix} 0 & 1 \\ v_0 - k^2 & 0 \end{pmatrix}$$

one finds that $J^2 = (v_0 - k^2)I$, where I is the unit 2×2 matrix, hence (see, *e.g.*, Ref. 7)

$$\exp(-LJ) = \begin{cases} \cosh(L\sqrt{v_0 - k^2})I - \frac{\sinh(L\sqrt{v_0 - k^2})}{\sqrt{v_0 - k^2}}J, & \text{if } v_0 - k^2 > 0, \\ \cos(L\sqrt{k^2 - v_0})I - \frac{\sin(L\sqrt{k^2 - v_0})}{\sqrt{k^2 - v_0}}J, & \text{if } v_0 - k^2 < 0, \\ I - LJ, & \text{if } v_0 - k^2 = 0. \end{cases} \quad (13)$$

On the other hand, from Eq. (2) we have

$$\psi(a) = A_1 + A_2, \quad \psi'(a) = ik(A_1 - A_2), \quad \psi(b) = B_1 + B_2, \quad \psi'(b) = ik(B_1 - B_2),$$

that is,

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -i/k \\ 1 & i/k \end{pmatrix} \begin{pmatrix} \psi(a) \\ \psi'(a) \end{pmatrix}, \quad \begin{pmatrix} \psi(b) \\ \psi'(b) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}. \quad (14)$$

(Note that Eqs. (14) correspond to the continuity conditions for ψ and ψ' at $x = a$ and $x = b$.)

Then, noting that

$$\frac{1}{2} \begin{pmatrix} 1 & -i/k \\ 1 & i/k \end{pmatrix} J \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} = \frac{1}{2ik} \begin{pmatrix} v_0 - 2k^2 & v_0 \\ -v_0 & -v_0 + 2k^2 \end{pmatrix},$$

from Eqs. (12)–(14) one finds that, for a rectangular potential barrier (or potential well)

$$V(x) = \begin{cases} 0, & \text{if } x < a \text{ or } x > b, \\ V_0, & \text{if } a \leq x \leq b, \end{cases} \quad (15)$$

the transfer matrix is given by

$$M = \begin{cases} \cosh(L\sqrt{v_0 - k^2}) I - \frac{\sinh(L\sqrt{v_0 - k^2})}{\sqrt{v_0 - k^2}} \frac{1}{2ik} \begin{pmatrix} v_0 - 2k^2 & v_0 \\ -v_0 & -v_0 + 2k^2 \end{pmatrix}, & \text{if } v_0 - k^2 > 0, \\ \cos(L\sqrt{k^2 - v_0}) I - \frac{\sin(L\sqrt{k^2 - v_0})}{\sqrt{k^2 - v_0}} \frac{1}{2ik} \begin{pmatrix} v_0 - 2k^2 & v_0 \\ -v_0 & -v_0 + 2k^2 \end{pmatrix}, & \text{if } v_0 - k^2 < 0, \\ I - \frac{ikL}{2} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}, & \text{if } v_0 - k^2 = 0. \end{cases} \quad (16)$$

Note that owing to the definitions of the amplitudes A_1 , A_2 , B_1 , and B_2 in terms of the exponentials $e^{\pm ik(x-a)}$ and $e^{\pm ik(x-b)}$, the transfer matrices (16) depend on a and b only through their difference $L = b - a$. The simplicity of the transfer matrices (16) contrasts with the complexity of the expressions for the reflection and transmission amplitudes obtained in the standard manner (see, *e.g.*, Ref. 2, chap. 5). Note also that even though we follow the conventions of Ref. 5, the transfer matrix (16) does not agree with the amplitudes given in Eq. (12) of Ref. 5.

It may also be noticed that, by allowing $\sqrt{v_0 - k^2}$ to become pure imaginary or taking the limit as $\sqrt{v_0 - k^2}$ goes to zero, from the first expression in (16) one can obtain the other two.

Furthermore, one can verify directly that, when k is real, the transfer matrices (16) are of the form $\begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}$, with $|\alpha|^2 - |\beta|^2 = 1$ and therefore they indeed belong to $SU(1,1)$. On the other hand, Eqs. (11)–(13) hold for k real or complex and since the trace of J is equal to zero for any value of k (even if $V(x)$ was not real), the determinant of $\exp(-LJ)$ is equal to 1; therefore, the transfer matrices (16) have determinant equal to 1 also when k is complex, though M no longer belongs to $SU(1,1)$.

The example considered in this section also allows us to illustrate the fact that making use of the transfer matrix one can find the energies of the bound states or the quasinormal modes, by considering pure imaginary or complex values of k , respectively.

In the case of the bound states of the potential well (15) with $V_0 < 0$, we have $E < 0$ and writing $k = i|k|$, from Eq. (2) we see that in order for the wave function to remain bounded, $B_2 = 0$ and $A_1 = 0$. Then Eq. (3) implies that M_{11} , the first entry of the diagonal of M , must be equal to zero. Since the determinant of the transfer matrix is equal to 1 (independent of the value of k), this last condition is equivalent to saying that the off-diagonal entries of M (which have opposite signs) must be equal to $+1$ or -1 . In the present case $v_0 - k^2 < 0$, and from the second line of Eq. (16) we have

$$\frac{\sin(L\sqrt{-|k|^2 - v_0})}{\sqrt{-|k|^2 - v_0}} \frac{v_0}{2|k|} = \pm 1,$$

which is equivalent to the conditions obtained in the textbooks (see, *e.g.*, Refs. 1,2).

The so-called quasinormal modes correspond to complex values of k for which there are no incident waves on the potential barrier but only outgoing waves. In this case the solution of the time-independent Schrödinger equation are of the form

$$\psi(x) = \begin{cases} A_2 e^{-ik(x-a)}, & x < a, \\ B_1 e^{ik(x-b)}, & x > b, \\ u(x), & a \leq x \leq b, \end{cases} \quad (17)$$

assuming that the real part of k is positive (*cf.* Eq. (2), A_1 and B_2 are equal to zero so that there are no ingoing waves on the barrier). Thus, as in the case of the bound states, we have $M_{11} = 0$ and, making use of the first expression in Eq. (16), we have

$$\cosh(L\sqrt{v_0 - k^2}) - \frac{\sinh(L\sqrt{v_0 - k^2})}{\sqrt{v_0 - k^2}} \frac{v_0 - 2k^2}{2ik} = 0$$

which can also be expressed in the form

$$\cosh(L\sigma) - \frac{\sinh(L\sigma)}{\sigma} \frac{\sigma^2 - k^2}{2ik} = 0, \quad (18)$$

with the definition $\sigma \equiv \sqrt{v_0 - k^2}$. Hence, $\sigma^2 + k^2 = v_0$. Following Chandrasekhar [8], we parameterize k and σ according to

$$k = Q \sin \alpha, \quad \sigma = Q \cos \alpha, \quad (19)$$

with $Q^2 = v_0$ and $Q \geq 0$ (assuming $v_0 \geq 0$). Substituting these expressions for k and σ into Eq. (18) we have

$$\cosh(L\sigma) - \sinh(L\sigma) \frac{Q^2 \cos^2 \alpha - Q^2 \sin^2 \alpha}{2iQ^2 \sin \alpha \cos \alpha} = 0,$$

which is equivalent to

$$\cosh(L\sigma) + i \sinh(L\sigma) \cot 2\alpha = 0. \quad (20)$$

Making use of the identities $\sin z = -i \sinh(iz)$, $\cos z = \cosh(iz)$, this last equation can be written as $\sinh(L\sigma) \cosh(i2\alpha) - \cosh(L\sigma) \sinh(i2\alpha) = 0$, which is equivalent to

$$\sinh(L\sigma - i2\alpha) = 0$$

and, therefore, $L\sigma - i2\alpha = in\pi$, where n is an integer. Then, letting $\alpha = \alpha_1 + i\alpha_2$ and $\sigma = \sigma_1 + i\sigma_2$, we have

$$L\sigma_1 = -2\alpha_2, \quad L\sigma_2 = 2\alpha_1 - n\pi. \quad (21)$$

From the relation $\sigma_1 + i\sigma_2 = Q \cos(\alpha_1 + i\alpha_2)$ [see Eq. (19)] we obtain

$$\sigma_1 = Q \cos \alpha_1 \cosh \alpha_2, \quad \sigma_2 = -Q \sin \alpha_1 \sinh \alpha_2 \quad (22)$$

and, combining Eqs. (21) and (22), it follows that

$$-2\alpha_2 = LQ \cos \alpha_1 \cosh \alpha_2, \quad 2\alpha_1 - n\pi = -LQ \sin \alpha_1 \sinh \alpha_2. \quad (23)$$

Hence,

$$\tan \alpha_1 \tanh \alpha_2 = \frac{2\alpha_1 - n\pi}{2\alpha_2}. \quad (24)$$

Similarly, from Eq. (19), we have $k_1 + ik_2 = Q \sin(\alpha_1 + i\alpha_2)$, that is,

$$k_1 = Q \sin \alpha_1 \cosh \alpha_2, \quad k_2 = Q \cos \alpha_1 \sinh \alpha_2$$

and, making use of Eqs. (23),

$$k_1 = -\frac{2\alpha_2 \tan \alpha_1}{L}, \quad k_2 = -\frac{2\alpha_2 \tanh \alpha_2}{L}. \quad (25)$$

By hypothesis, $k_1 \geq 0$ and $Q \geq 0$, therefore from Eqs. (24) and (25) it follows that

$$\begin{aligned} \text{if } \alpha_2 > 0 &\Rightarrow \tan \alpha_1 \leq 0, \quad 2\alpha_1 - n\pi \leq 0 \Rightarrow n > 0, \quad \frac{\pi}{2} \leq \alpha_1 \leq \pi, \\ \text{if } \alpha_2 < 0 &\Rightarrow \tan \alpha_1 \geq 0, \quad 2\alpha_1 - n\pi \geq 0 \Rightarrow n \leq 0, \quad 0 \leq \alpha_1 \leq \frac{\pi}{2}. \end{aligned}$$

Given a solution, α_1, α_2 , of Eqs. (23), the values of k_1 and k_2 are determined by means of Eqs. (25).

Since the time-independent Schrödinger equation (1) is obtained assuming that the wave function has a time dependence of the form $\exp(-iEt/\hbar)$. When k is complex, E has a negative imaginary part for $k_1 > 0$ [k_2 is negative, see Eq. (25)] that produces an exponential decay in time.

Denoting by $M^{(a,b)}$ the matrix appearing in Eq. (3), we have the relation

$$M^{(a,c)} = M^{(a,b)} M^{(b,c)},$$

for any value of c . This relation together with Eq. (16) allow us to readily find the transfer matrix (or, equivalently, the transmission and reflection amplitudes) for any piecewise constant potential and from the condition $M_{11} = 0$, the bound states and quasinormal modes can then be obtained, though the expressions will be even more involved than the ones considered here.

4. Reflection and transmission of electromagnetic waves

The behavior of a linearly polarized electromagnetic plane wave normally incident on a slab of dielectric material can be found following a procedure similar to that employed in the preceding section. For plane monochromatic waves propagating along the x -axis with the electric field parallel to the y -axis in a homogeneous dielectric medium, the wave equation reduces to

$$\frac{d^2 E_y}{dx^2} + k^2 E_y = 0, \tag{26}$$

where $k = n\omega/c$, n is the refractive index of the medium and ω is the frequency of the wave. Equation (26) can be expressed as the first-order equation

$$\frac{d}{dx} \begin{pmatrix} E_y \\ dE_y/dx \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -k^2 & 0 \end{pmatrix} \begin{pmatrix} E_y \\ dE_y/dx \end{pmatrix}, \tag{27}$$

which is of the form (11) with $v = 0$; hence,

$$\begin{pmatrix} E_y(a) \\ dE_y/dx|_{x=a} \end{pmatrix} = \widetilde{M} \begin{pmatrix} E_y(b) \\ dE_y/dx|_{x=b} \end{pmatrix},$$

where [see Eqs. (12) and (13)]

$$\widetilde{M} = \cos(kL) I - \frac{\sin(kL)}{k} \begin{pmatrix} 0 & 1 \\ -k^2 & 0 \end{pmatrix}$$

and $L = b - a$.

If the slab is bounded by the planes $x = a$ and $x = b$ and, for instance, surrounded by vacuum, Eq. (26) has solutions of the form

$$E_y = \begin{cases} A_1 e^{ik_0(x-a)} + A_2 e^{-ik_0(x-a)}, & \text{for } x < a, \\ B_1 e^{ik_0(x-b)} + B_2 e^{-ik_0(x-b)}, & \text{for } x > b, \end{cases} \quad (28)$$

where $k_0 \equiv \omega/c$. Faraday's law imply that the z -component of the magnetic field is proportional to dE_y/dx and, therefore, the continuity of the tangential components of the fields at the boundary of the slab amounts to the continuity of E_y and dE_y/dx and from Eq. (28) we see that

$$E_y(a) = A_1 + A_2, \quad \frac{dE_y}{dx}(a) = ik_0(A_1 - A_2), \quad E_y(b) = B_1 + B_2, \quad \frac{dE_y}{dx}(b) = ik_0(B_1 - B_2),$$

thus, proceeding as in the previous section we obtain the relation

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = M \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} \quad (29)$$

with the transfer matrix

$$M = \cos(kL) I - \frac{\sin(kL)}{k} \frac{i}{2k_0} \begin{pmatrix} k_0^2 + k^2 & -k_0^2 + k^2 \\ k_0^2 - k^2 & -k_0^2 - k^2 \end{pmatrix}, \quad (30)$$

which is related to the transmission and reflection amplitudes as in Eq. (9). It may be noticed that, also in the present case, the transfer matrix (30) belongs to $SU(1,1)$ for k real and that the determinant of M is equal to 1 even if k is complex (which would correspond to a nonzero conductivity).

Acknowledgment

One of the authors (I.R.G.) thanks the Vicerrectoría de Investigación y Estudios de Posgrado of the Universidad Autónoma de Puebla for financial support through the programme “La ciencia en tus manos.”

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